The target problem with evanescent subdiffusive traps

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We calculate the survival probability of a stationary target in one dimension surrounded by diffusive or subdiffusive traps of time-dependent density. The survival probability of a target in the presence of traps of constant density is known to go to zero as a stretched exponential whose specific power is determined by the exponent that characterizes the motion of the traps. A density of traps that grows in time always leads to an asymptotically vanishing survival probability. Trap evanescence leads to a survival probability of the target that may be go to zero or to a finite value indicating a probability of eternal survival, depending on the way in which the traps disappear with time.

I. INTRODUCTION

The traditional *trapping* problem involves diffusive (Brownian) particles (A) that wander in a medium doped with static traps (B) and disappear when they meet [1, 2, 3, 4]. In the traditional *target* problem [5, 6, 7], on the other hand, one has static A particles and mobile traps. Both of these problems are described by the "reaction" $A + B \rightarrow B$, but in one case the A's move and the B's stand still, while in the other the B's move while the A's are stationary. Both of these problems have a long and active history in the literature. They not only represent experimentally observable phenomena, but they have served as a testbed for theoretical and numerical studies and as a starting point for the formulation of models for more complex systems that have only recently been successfully solved analytically. For example, the survival probability of an A particle in a medium of B particles when *both* species are diffusive, first investigated numerically in the seminal work of Toussaint and Wilczek [8], was only partially solved analytically [9, 10] until the recent full (asymptotic) solution in one dimension [11, 12, 13, 14]. These results have also recently been generalized to subdiffusive species [15]. The survival probability of A particles in the reactions $A + A \rightarrow A$ and $A + A \rightarrow 0$ in one dimension when A is mobile is also of relatively recent vintage in the history of such analytic solutions [4, 16, 17].

The purpose of this paper is to extend the one-dimensional target problem calculations for both diffusive and subdiffusive traps to the case of traps that themselves disappear in time according to some survival probability function of their own (e.g., exponential or power law). The decay of the moving traps with time of course increases the survival probability of the stationary target, and the interesting questions concern the interplay of the time dependences of the movement and decay of the traps. A related problem was considered in [18], where diffusive particles A and traps B and C undergoing the explicit reactions (a) $A + B \rightarrow B$, $B + C \rightarrow C$, and (b) $A + B \rightarrow B$, $B + C \rightarrow 0$ were considered using entirely different methods. Our methods are equally applicable to trap densities that increase with time, but this problem is less interesting because it necessarily leads to the eventual demise of the target.

A common characterization of the diffusive motion of a particle is through its mean square displacement for large t,

$$\langle x^2(t) \rangle \sim \frac{2K_\gamma}{\Gamma(1+\gamma)} t^\gamma. \tag{1}$$

Here K_γ is the (generalized) diffusion constant, and γ is the exponent that characterizes normal ($\gamma = 1$) or anomalous ($\gamma \neq 1$) diffusion. In particular, the process is sudiffusive when $0 < \gamma < 1$. Subiffusive processes are ubiquitous in nature [19, 20, 21, 22, 23, 24], and are particularly useful for understanding transport in complex systems [3, 25].

The problem considered in this paper is a special case of a broad class of reaction-*subdiffusion* processes that have been studied over the past decades. One approach that has been used to study these processes is based on the continuous time random walk (CTRW) theory with waiting-time distributions between steps that have broad long-time tails and consequently infinite moments, $\psi(t) \sim t^{-1-\gamma}$ for $t \rightarrow \infty$ with $0 < \gamma < 1$. Another approach is based on the fractional diffusion equation, which describes the evolution of the probability density $P(x,t)$ of finding the particle at position x at time t by means of the fractional partial differential equation (in one dimension) [7, 19, 26, 27, 28, 29]

$$\frac{\partial}{\partial t} P(x,t) = K_\gamma \, _0D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} P(x,t), \tag{2}$$

where $_0D_t^{1-\gamma}$ is the Riemann-Liouville operator,

$$_0D_t^{1-\gamma} P(x,t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t dt' \frac{P(x,t')}{(t-t')^{1-\gamma}}. \tag{3}$$

In this paper we study the one-dimensional target problem for a static particle A subject to attack by diffusive or subdiffusive traps B that may die before reaching the target A [18]. For this purpose, we generalize the ideas of Bray and Blythe [11], and of our own work [15] based on a fractional diffusion equation approach. While recent work shows that a simple generalization of reaction-diffusion to reaction-subdiffusion equations in which the reaction and subdiffusion terms are assumed to enter additively is not valid in some cases [30], this is not a difficulty in our particular application. The difficulties do not arise when the reaction process can be translated into a static boundary value problem, which is the case for the target (as well as the trapping) problem [28].

In some cases, asymptotic anomalous diffusion behavior can be found from corresponding results for normal diffusion via the simple replacement of t by t^γ. This can be understood from a CTRW perpective because the average number of jumps n made by a subdiffusive walker up to time t scales as $\langle n \rangle \sim t^\gamma$ and, in many instances the number of jumps is the relevant factor that explains the behavior of the system. The simple replacement result is evidence of "subordination" (see Secs. 5 and 7.2 of [6]). However, there are other instances where the behavior of subdiffusive systems cannot be found in this way. A simple example is the survival probability of subdiffusive particles in the trapping problem (see Sec. 5 of [6]). In particular, for systems where competing processes (motion toward target and death) occur according to different temporal rules, such a replacement becomes ambiguous. This is the case for the problem considered here.

While our analytic results are based on the fractional diffusion equation formalism, our numerical simulations are based on a CTRW algorithm. These two renditions of the problem are expected to differ if trapping events are likely in a small number of steps, that is, if the initial density of traps is too high. On the other hand, if the initial trap density is too low, then the simulations to produce valid statistics would take inordinately long because trapping events are rare and because the system has to be sufficiently large to include many particles. We note this as a caveat for our subsequent comparisons.

In Sec. II we present an integral equation for the survival probability, which we reduce to quadrature in Sec. III. The resulting integral is explicitly evaluated for exponentially decaying trap densities (including a stretched exponential decay), as well as for trap densities that decay as a power law. Not surprisingly, we find that a sufficiently rapid decay of the trap density leads to a finite asymptotic survival probability of the target. Comparisons of our results with numerical simulations are also shown in this section. A summary and some conclusions are presented in Sec. IV.

II. INTEGRAL EQUATION FOR THE SURVIVAL PROBABILITY

We consider a finite interval L containing $N = \rho L$ mobile traps B of constant density ρ initially distributed at random, and a single immobile A particle at the origin. Following the approach of Bray et al. [14] for diffusive traps and our generalization of this approach to the subdiffusive case [15], we write the survival probability of A as $P(t) = \exp\{-\mu_0(t)\}$, where $\mu_0(t)$ is to be determined. To find this function, one calculates in two ways the probability density to find a B particle at the origin at time t,

$$\rho = \int_0^t dt' \dot{\mu}_0(t') G(t - t'). \qquad (4)$$

That the left side is this probability density is obvious. On the right side one has the renewal theory expression where $\dot{\mu}_0(t')dt' = (-\dot{P}/P)dt'$ is the probability that a B particle intersected A in the time interval $(t', t' + dt')$ for the first time, and the propagator $G(t - t')$ is the probability density for this particular B to be at the origin at time t. In one dimension it is given by [31, 32]

$$
\begin{aligned}
G(t) &= \frac{1}{\sqrt{4\pi K_\gamma t^\gamma}} H_{1,2}^{2,0}\left[0 \left|\begin{array}{l} (1 - \gamma/2, \gamma/2) \\ (0,1), (1/2, 1) \end{array}\right.\right] \\
&= \frac{1}{\sqrt{4 K_\gamma t^\gamma} \Gamma\left(1 - \frac{\gamma}{2}\right)},
\end{aligned} \qquad (5)
$$

where $H_{1,2}^{2,0}$ is Fox's H-function, whose value at the given arguments we have used to write the last equality. In a different context than the target problem, Bray et al. [14] generalized their approach to a time-dependent density $\rho(t)$ of B. They argue that in place of Eq. (4) one now has

$$\rho(t) = \int_0^t dt' \frac{\rho(t)}{\rho(t')} \dot{\mu}_0 G(t - t'), \qquad (6)$$

that is,

$$1 = \int_0^t dt' \frac{\dot{\mu}_0}{\rho(t')} G(t - t'). \qquad (7)$$

This is the basic equation to be considered in this paper.

III. THE SURVIVAL PROBABILITY

To calculate the survival probability of particle A, we rewrite Eq. (7) explicitly as

$$\sqrt{4 K_\gamma} = \frac{1}{\Gamma(1 - \gamma/2)} \int_0^t dt' \frac{\Omega(t')}{(t - t')^{\gamma/2}}, \qquad (8)$$

where we have multiplied both sides by $\sqrt{4 K_\gamma}$, and where we have introduced

$$\Omega(t) = \frac{\dot{\mu}_0(t)}{\rho(t)}. \qquad (9)$$

Equation (8) is an equation of Abel of the first kind [33, 34],

$$f(t) = \frac{1}{\Gamma(1-\gamma/2)} \int_0^t dt' \frac{\Omega(t')}{(t-t')^{\gamma/2}}, \qquad (10)$$

with $f(t) = \sqrt{4K_\gamma}$. The solution of this classic equation is well known (see Sec. 12 in [33] or Eqs. (2.5a) and (2.5b) in [34]),

$$\Omega(t) = {}_0D_t^{1-\gamma/2} f(t)$$
$$= \frac{1}{\Gamma(\gamma/2)} \int_0^t dt' \frac{\dot{f}(t')}{(t-t')^{1-\gamma/2}} + f(0^+) \frac{t^{\gamma/2-1}}{\Gamma(\gamma/2)}. \qquad (11)$$

Here, as earlier, ${}_0D_t^{1-\gamma/2}$ is the Riemann-Liouville fractional derivative. In our case $f(t) = \sqrt{4K_\gamma}$ is constant, so that

$$\Omega(t) = \frac{\dot{\mu}_0(t)}{\rho(t)} = \frac{\sqrt{4K_\gamma}}{\Gamma(\gamma/2)} t^{\gamma/2-1}. \qquad (12)$$

It then follows that

$$\mu_0(t) = \frac{\sqrt{4K_\gamma}}{\Gamma(\gamma/2)} \int_0^t dz \rho(z) z^{\gamma/2-1}, \qquad (13)$$

which provides a general solution to our problem for any $\rho(t)$. While Eq. (13) applies to trap densities that grow or that decrease or even oscillate in time, the case of evanescent traps is the more interesting and the one we choose to focus on.

As a reminder, we note that for traps of a constant density $\rho(t) = \rho_0$ the survival probability is given by

$$P(t) = \exp\left(\frac{\sqrt{4K_\gamma} \rho_0 t^{\gamma/2}}{\Gamma(1+\gamma/2)}\right). \qquad (14)$$

As a benchmark, we show in Fig. 1 a typical comparison of this result with simulation results. The agreement is clearly good, although a lower initial density run for a longer time would lead to even better agreement.

A. Exponentially decaying trap density

Suppose that the traps have a finite lifetime τ and decay exponentially, as in a unimolecular reaction, $\rho(t) = \rho_0 \exp(-t/\tau)$. The integral in Eq. (13) immediately leads to the solution

$$\mu_0(t) = \ell_\gamma \rho_0 \left(1 - \frac{\Gamma(\gamma/2, t/\tau)}{\Gamma(\gamma/2)}\right), \qquad (15)$$

where $\Gamma(b,x)$ is an incomplete Gamma function, and

$$\ell_\gamma \equiv (4K_\gamma \tau^\gamma)^{1/2}. \qquad (16)$$
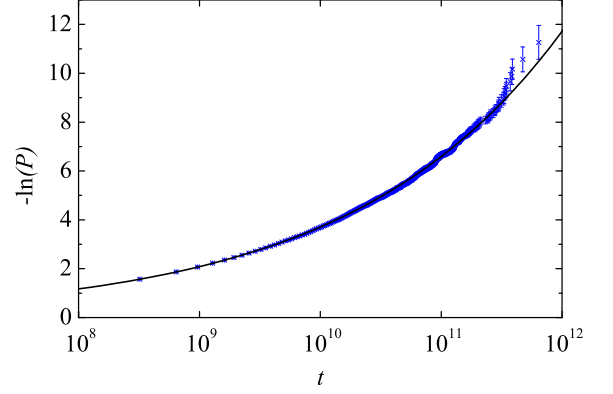
FIG. 1: (Color online) $\mu_0(t) = -\ln P(t)$ vs t for non-evanescent traps as given in Eq. (14) (solid line) and simulations (symbols along with error bars). Parameter values are $\gamma = 1/2$, $\rho_0 = 0.01$, $K_\gamma = 1/(2\sqrt{\pi})$.

When $\gamma = 1$, i.e., when the traps are diffusive, this reduces to

$$\mu_0(t) = \ell_1 \rho_0 \text{erf}(\sqrt{t/\tau}). \qquad (17)$$

For arbitrary $\gamma < 1$, the survival probability of the target in the presence of the subdiffusive traps with finite lifetime thus is

$$P(t) = \exp\left[-\ell_\gamma \rho_0 \left(1 - \frac{\Gamma(\gamma/2, t/\tau)}{\Gamma(\gamma/2)}\right)\right]. \qquad (18)$$

The interesting result here is that the funtion $\mu_0(t)$ goes to the constant $\mu_0(\infty) = \ell_\gamma \rho_0$ and not to infinity as $t \to \infty$. Therefore the survival probability does not vanish with increasing time,

$$P(t) \to \exp\left[-\ell_\gamma \rho_0 \left(1 - \frac{e^{-t/\tau}}{\Gamma(\gamma/2)(t/\tau)^{1-\gamma/2}}\right)\right]. \qquad (19)$$

We note that ℓ_γ is a characteristic distance that measures the root mean square displacement of the traps during their decay time τ. Therefore $\mu_0(\infty) = \ell_\gamma \rho_0$ is the ratio of this average displacement to the average initial distance ρ_0^{-1} between traps. This finite asymptotic survival probability, $P(\infty) = \exp(-\ell_\gamma \rho_0)$, displays reasonable qualitative features: it increases with decreasing trap lifetime τ, and it decreases with increasing initial trap density ρ_0. That there is a finite asymptotic survival probability reflects the fact that if the traps disappear sufficiently rapidly (which they do if they disappear exponentially while the traps move diffusively or subdiffusively), then many traps disappear before they can reach the particle, and there is a finite probability that the particle remains forever "safe."

The next two figures show the comparison of simulation results with our analytic outcome. First, in Fig. 2
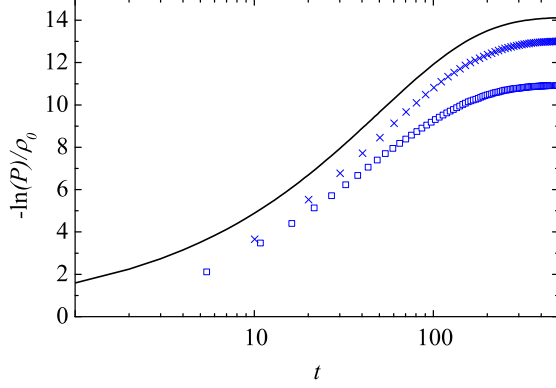
FIG. 2: (Color online) $\mu_0(t)/\rho_0 = -\ln P(t)/\rho_0$ vs t for exponentially evanescent traps. Solid line: Eq. (17). Squares: simulation results for a high initial density $\rho_0 = 0.1$. X's: simulation results for a lower initial density $\rho_0 = 0.01$. Other parameter values are $\gamma = 1$, $\tau = 100$, and $K_1 = D = 1/2$. Asymptotic value: $\mu_0(\infty) = \ell_1 \rho_0 = \sqrt{2}$.

FIG. 3: (Color online) $\mu_0(t) = -\ln P(t)$ vs t for exponentially evanescent traps of a lower initial density $\rho_0 = 0.01$. Solid line: Eq. (18). Symbols: simulation results (there are error bars on the symbols but they are too small to see clearly). Other parameter values are $\gamma = 1/2$, $\tau = 10^8$, and $K_\gamma = 1/(2\sqrt{\pi})$. Asymptotic value: $\mu_0(\infty) = \ell_{1/2} \rho_0 = 1.06225$.

we illustrate our earlier caveat, that agreement cannot be expected if the initial density of traps is too high and the extinction rate of the traps is large, and that the agreement improves with lower initial density. The disagreement is clear and can be traced exactly to the early time trapping events that cumulatively affect the survival probability. Fig. 3 shows typical results for the lower initial density of traps and a more slowly decaying trap density, where the agreement between analytic results and simulations is clearly very good.

Finally, it is straightforward to extend the results of this section to trap densities that decay as a stretched exponential, $\rho(t) = \rho_0 \exp[-(t/\tau)^\alpha]$. The integral (13) is still straightforward and gives

$$\mu_0(t) = \frac{\ell_\gamma \rho_0 \Gamma(\gamma/2\alpha)}{\alpha \Gamma(\gamma/2)} \left(1 - \frac{\Gamma(\gamma/2\alpha, (t/\tau)^\alpha)}{\Gamma(\gamma/2\alpha)}\right), \quad (20)$$

which reduces to Eq. (15) when $\alpha = 1$. The asymptotic finite survival probability then is

$$P(t) \to \exp\left[-\ell_\gamma \rho_0 \frac{\Gamma(\gamma/2\alpha)}{\alpha \Gamma(\gamma/2)} \left(1 - \frac{e^{(-t/\tau)^\alpha}}{\Gamma(\gamma/2\alpha)(t/\tau)^{\alpha(1-\gamma/2)}}\right)\right] \cdot \tag{21}$$

An interesting interplay of γ and α should be noted: there are values of α and γ for which the survival probability of the target when the trap density decays as a stretched exponential ($\alpha < 1$) is actually greater than with an exponential decay ($\alpha = 1$). This seemingly counterintuitive behavior is connected with the reversal of time inequalities, i.e., with the fact that $(t/\tau)^\alpha$ is greater (smaller) than (t/τ) when t is smaller (greater) than τ.

B. Power law decaying trap density

Suppose now that the trap density decays as a power law as might happen, for instance, if there is a process of trap-trap annihilation. The trap density at long times then decreases as $\rho(t) \sim t^{-\beta}$ and it is to be expected that the target survival probability (and, in particular, whether it is asymptotically vanishing or finite) depends sensitively on the relation between the exponents β and γ. We expect that for sufficiently large β the target will again have a finite probability of surviving forever.

To find a closed expression for the survival probability we need to specify $\rho(t)$ for all times, not just asymptotically, and we choose

$$\rho(t) = \frac{\rho_0}{(1 + t/\tau)^\beta}. \tag{22}$$

With this form, the integral (15) can be carried out exactly, to give

$$\mu_0(t) = \frac{\ell_\gamma \rho_0}{\Gamma(\gamma/2)} B_{\frac{t}{(\tau+t)}}(\gamma/2, \beta - \gamma/2) \tag{23}$$

for all β, where B is the incomplete Beta function [36, 37]

$$B_\alpha(z, w) = \int_0^\alpha dt \, t^{z-1}(1-t)^{w-1} \quad \text{with } \Re(z) > 0. \tag{24}$$

Equation (1) tells us that the typical length explored by a (living) trap grows with time as $\langle x^2(t) \rangle^{1/2} \sim t^{\gamma/2}$. On the other hand, the mean distance between traps grows as $\rho^{-1} \sim t^\beta$. It thus stands to reason that the asymptotic survival probability depends sensitively on

the relative magnitudes of β and $\gamma/2$. To present more explicit results in this long-time regime we distinguish three cases.

Case 1: $\beta > \gamma/2$. In this case Eq. (23) can be written as

$$\mu_0(t) = \frac{\ell_\gamma \rho_0}{\Gamma(\gamma/2)} B(\gamma/2, \beta - \gamma/2) I_{\frac{t}{(\tau+t)}}(\gamma/2, \beta - \gamma/2). \quad (25)$$

Here $B(z, w)$ is the Beta function (where the requirement $\Re(z) > 0$ and $\Re(w) > 0$ places us in the "Case 1" regime), and $I_x(z, w)$ is the regularized incomplete Beta function as defined in Sec. 6.6.2 (pg. 263) of [37]. Using the property 6.6.3 in [37] we can set $I_x(a, b) = 1 - I_{1-x}(b, a)$, and applying the relation 26.5.5 in [37] we can then write the asymptotic result

$$I_{\frac{t}{(\tau+t)}}(\gamma/2, \beta - \gamma/2) = 1 - \frac{(t/\tau)^{\gamma/2 - \beta}}{(\beta - \gamma/2) B(\beta - \gamma/2, \gamma/2)} + \cdots. \quad (26)$$

Consequently, recognizing the relation between the Beta function and the Gamma function, as $t \to \infty$ we arrive at the asymptotic result

$$\mu_0(t) \to \ell_\gamma \rho_0 \left(\frac{\Gamma(\beta - \gamma/2)}{\Gamma(\beta)} - \frac{(t/\tau)^{\gamma/2 - \beta}}{(\beta - \gamma/2)\Gamma(\gamma/2)} + \cdots \right). \quad (27)$$

The survival probability thus approaches (via a power law decay of the exponent) the finite asymptotic value

$$P(t \to \infty) = \exp\left(-\ell_\gamma \rho_0 \frac{\Gamma(\beta - \gamma/2)}{\Gamma(\beta)} \right). \quad (28)$$

Figure 4 illustrates this result along with numerical simulations for comparison.

Case 2: $\beta < \gamma/2$. In this case the integrand in Eq. (13) goes to zero more slowly than $1/t$ for $t \to \infty$, so that a simple asymptotic analysis of the integral (13) readily establishes that $\mu_0(t)$ goes to infinity with increasing time as

$$\mu_0(t) \to \frac{\ell_\gamma \rho_0}{(\gamma/2 - \beta)\Gamma(\gamma/2)} \left(\frac{t}{\tau} \right)^{\gamma/2 - \beta} + \ldots, \quad (29)$$

so that the survival probability vanishes at long times as a stretched exponential,

$$P(t) \to \exp\left(-\frac{\ell_\gamma}{(\gamma/2 - \beta)\Gamma(\gamma/2)} (t/\tau)^{\gamma/2 - \beta} \right). \quad (30)$$

Analytic and simulation results for this case are shown in Fig. 5.

Case 3: $\beta = \gamma/2$. This is the marginal case, and the incomplete Beta function (24) can be rewritten as a hypergeometric function,

$$\mu_0(t) = \frac{\ell_\gamma \rho_0 (t/\tau)^\beta}{\beta \Gamma(\gamma/2)} \, {}_2F_1(\beta, \beta, 1 + \beta, -t/\tau)$$

$$= \frac{\ell_\gamma \rho_0}{\Gamma(\gamma/2)} \ln(t/\tau) + \ldots \quad \text{as } t \to \infty. \quad (31)$$
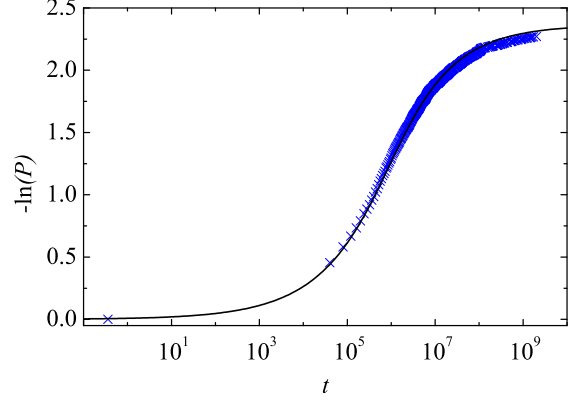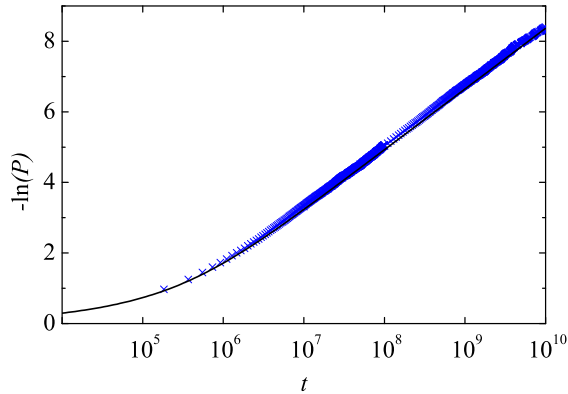

FIG. 4: (Color online) $\mu_0(t) = -\ln P(t)$ vs t for power law evanescent traps with $\beta > \gamma/2$ ("Case 1"). Parameter values are $\gamma = 0.75$, $\beta = 0.8$, $\rho_0 = 0.01$, $\tau = 10^6$, and $K_\gamma = 1/(2\sqrt{\pi})$. Asymptotic value: $\mu_0(\infty) = \ell_{3/4}\rho_0 = 2.36549$. Solid line: Eq. (23). Symbols: simulation results.
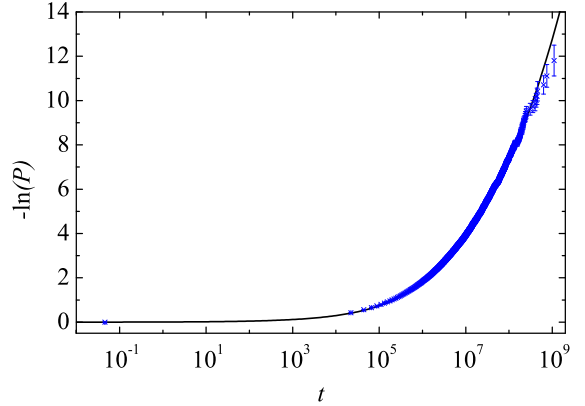
FIG. 5: (Color online) $\mu_0(t) = -\ln P(t)$ vs t for power law evanescent traps with $\beta < \gamma/2$ ("Case 2"). Parameter values are $\gamma = 0.8$, $\beta = 0.2$, $\rho_0 = 0.01$, $\tau = 10^6$, and $K_\gamma = 1/(2\sqrt{\pi})$. Solid line: Eq. (23). Symbols: simulation results along with error bars.

The survival probability thus decays as an inverse power,

$$P(t \to \infty) \to (t/\tau)^{-\ell_\gamma \rho_0/\Gamma(\gamma/2)}. \quad (32)$$

Results for the marginal case are shown in Fig. 6.

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